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FIELD	GROUP	SUB-GROUP	

19. ABSTRACT (Continue on reverse if necessary and identify by block number)

A Gordon Research Conference on Computational Chemistry was held at Plymouth State College 4-8 July 1988. There were 150 attendees. A broad range of topics were covered in some depth: macromolecular simulations (molecular dynamics) of proteins and lipids, charge polarizability, protein folding, free energy perturbation calculations, conformational analysis of drug-sized molecules, molecular mechanics, pharmacophore mapping, computer-assisted molecular design, distance geometry, applied quantum mechanics at the ab initio and semiempirical levels, quantitative structure-property relationships, and electronic and conformational properties of inorganics and solids. There were 62 poster papers on diverse topics.

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1988 GORDON RESEARCH CONFERENCE ON COMPUTATIONAL CHEMISTRY

Final Progress Report

Interest in the second Computational Chemistry Gordon Conference was commensurate with the high activity in this important area of research. The conference was held at Plymouth State College (South Site), Plymouth, New Hampshire, July 4-8, 1988. Based on responses we received, the meeting was very worthwhile and beneficial to the participants, and the facilities were satisfactory.

There were 240 applicants. Fortunately we were able to get the attendance limit raised from 135 to 150 which contributed to a more successful conference. The high number of applicants is remarkable in light of the fact that there are about 30 other meetings and symposia, almost all of which are new this year, covering one or more aspects of computational chemistry.

The demographics of those accepted to the conference closely paralleled the demographics of applicants (similar to the way Drs. Boyd and Lipkowitz organized the first conference in 1986). Representatives from 104 organizations were accepted: 50% of the attendees were from 48 colleges and universities, 35% were from 41 pharmaceutical, chemical, and hardware/software companies, 15% were from 15 government and private laboratories. 15% of the participants were from outside the US representing 15 countries. The demographics produced a cross-fertilization of subspecialties engendering growth of the field. About 2/3 of the attendees were not at the 1986 conference, thereby bringing in fresh perspectives.

Consistent with the objectives set for this conference when it first met in 1986, many facets of computational chemistry were represented in the program and a proper balance between methodology and applications was achieved. Theory/methodology and applications must go hand in hand. Theory per se is of little interest if its use is not demonstrated. Conversely, specific applications (most of which are in Computer-Assisted Molecular Design and three-dimensional structure elucidation) are of interest to a narrow segment of any audience unless the methodology is discussed in sufficient detail to show wide applicability.

A broad range of topics were covered in some depth: macromolecular simulations (molecular dynamics) of proteins and lipids, charge polarizability, protein folding, free energy perturbation calculations, conformational analysis of drug-sized molecules, molecular mechanics, pharmacophore mapping, computer-assisted molecular design, distance geometry, applied quantum mechanics at the ab initio and

semiempirical levels, quantitative structure-property relationships, and electronic and conformational properties of inorganics and solids.

The widely based discussions following each of the 26 invited talks indicate that a good vigorous mix of interests were represented at the conference. Private comments indicated that only one or two talks, such as at the distance geometry session, were too specialized and should have been aimed at a broader audience.

The quality and freshness of the 62 poster papers were excellent. The range of topics was diverse enough to appeal to a wide variety of interests. Several people commented that they liked the way the program was organized with two full evening poster sessions. The two sessions were purposely designed so as not to have all the quantum mechanical papers together, or all the molecular mechanics papers together, etc. The attendees appreciated this arrangement because it gave presenters on one night an opportunity to see other posters on their field on the other night. Those presenting posters remarked that the discussions evoked were very good.

The question of whether to have the Computational Chemistry conference meet again in 1989 or 1990 was discussed at a plenary session. By overwhelming vote, it was decided that the conference should meet again in 1990. Despite the uncertain future of the Gordon Conference on Quantitative Structure-Activity Relationships (QSAR), a conference which in recent years had trended toward molecular modeling, most of the attendees favored continuing with the biennial meeting of the Computational Chemistry conference. Regarding the 90 individuals unable to attend because of the size limit on Gordon Conferences, less than 10 wrote or telephoned the chairmen to express their interest in having the conference meet every year.

The advantage of academic/industrial/government collaboration is one of the reasons the conference was set up with one chairman from academia and one from an industrial/government laboratory. Professor William L. Jorgensen (Purdue) and Dr. John McKelvey (Kodak) were elected 1990 Chairman and Vice-chairman, respectively.

An Advisory Committee consisting of past chairmen, Dr. Donald B. Boyd (Lilly), Professor Kenneth B. Lipkowitz (IUPUI), and Professor Peter Kollman (UCSF), will provide assistance and counsel to the new chairmen.

The duties of the Chairman will be to invite the speakers and discussion leaders, to handle the applications for attendance, and to prepare the program and reports. The

Vice-Chairman will be responsible for organizing the two poster sessions. The Chairman and Vice-Chairman will share the responsibility to apply for funding to support the conference. In order to provide continuity and rotate the chairmanship between academic and industrial representatives, the Vice-Chairman will assume the chairmanship at the following conference. Thus at the 1990 conference the new Vice-Chairman to be elected will be from academia.

We thank the following organizations for generous and essential support of and commitment to the conference: Gordon Research Conference Board of Trustees, Air Force Office of Scientific Research, Office of Naval Research, Quantum Chemistry Program Exchange (Indiana University), Eli Lilly and Company, and the University of California at San Francisco.

In the future, the Gordon Conference Office should implement a system so that those applicants not accepted receive a notification that their application was not approved by the Selection Committee. The present system of notification is inadequate. Although all applicants are sent a slip that their application was received in the mail, only those individuals accepted hear anything further from the office. This causes the chairmen (and Gordon Conference office) to be burdened with many telephone calls from people anxiously awaiting acceptance. For our conference, one of the chairmen took it upon himself to send out explanatory letters to those not accepted about four weeks before the conference.

"Not-accepted" notifications should be sent out by the Gordon Conference office when the chairman knows he will not or cannot accept someone. There should be an option on the weekly lists that the chairmen receive to check when they want the "not-accepted" notification sent.

Typically at a Gordon Conference, it is possible to accept 5-10 additional applicants the last week or two before the meeting when those previously accepted decide not to register. One of us wrote letters reminding those already accepted to inform us if they had changed their plans about attending. These letters did stimulate some responses. Again it would be helpful if the Gordon Conference office would send out reminders like this.

Donald B. Boyd and Peter Kollman, Co-chairmen
July 21, 1988

Program

GORDON RESEARCH CONFERENCE
on
Computational Chemistry

Donald B. Boyd and Peter Kollman, Co-chairmen

Boyd Hall, Plymouth State College, Plymouth, New Hampshire
July 4-8, 1988

July , 1988
Monday Morning 9:00 a.m. - 12:20 p.m.

Donald B. Boyd, Eli Lilly and Company
Peter Kollman, University of California, San Francisco
Introductory Remarks.

John J. Wendeloski, Dupont
Session Chairman and Discussion Leader
Macromolecular Simulations.

Axel T. Brunger, Yale University
Computational Tools for Structural Biology.

Coffee break 10:20 - 10:50 a.m.

Terry R. Stouch, Naval Research Laboratory
Molecular Dynamics Simulations of Simple Lipid Systems.

Wilfred F. van Gunsteren, University of Groningen
On Comparing Computer Simulations of Macromolecules with Experimental Data.

Monday Evening Poster Session
7:30 p.m. - 9:30 p.m.

Jeffry D. Madura, University of Houston
B. Montgomery Pettitt
J. Andrew McCammon
1. Determination of Transition State Geometries and Relative Free Energies of Activation in Condensed Phase.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

James R. Damewood, Jr., University of Delaware
Wolfgang C. F. Muehlbauer
2. Calculation of Intermolecular Potential Energy Surfaces Using Modified Molecular Mechanics Techniques.

Lee F. Kuyper, Burroughs Wellcome Company
Kenneth M. Merz, Jr., University of California, San Francisco
Peter A. Kollman
3. Relative Solvation Free Energies of Benzene, Anisole, and 1,2,3-Trimethoxybenzene: Theoretical and Experimental Analysis.

Salvatore Profeta, Jr., Glaxo Inc., Research Triangle Park
V. N. Balaji, Allergan
4. Conformational Energy Mapping Using MM2: Utility and Validity of Variable Energy Convergence Criteria With Applications to 2-D Energy Maps for Peptides and Drug Molecules.

Jerry A. Boatz, North Dakota State University
Mark S. Gordon
5. Decomposition of Normal Coordinate Vibrational Frequencies.

Mark S. Gordon, North Dakota State University
Kiet Nguyen
Larry P. Davis, Air Force Office of Scientific Research
Larry W. Burggraf
Krishnan Raghavachari, AT&T Bell Laboratories
6. Theoretical Analysis of the Reaction $Si^+ + SiH_3CH_3$.

Kim K. Baldridge, North Dakota State University
Mark S. Gordon
7. Illustration of Electronic Structure-Dynamics Interface.

Krzysztof Kuczera, Harvard University
John Kuriyan
Martin Karplus
8. Molecular Dynamics of Myoglobin.

J. Phillip Bowen, University of North Carolina at Chapel Hill
Vikram Reddy, Center for Disease Control
Donald G. Patterson, Jr.
Norman L. Allinger, University of Georgia
9. Molecular Mechanics Treatment of Halogenated Dibenzo-p-dioxins and Dibenzofurans: MM2 Parameters for Aromatic Halides, Divinyl Ethers, and Related Compounds.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

Kerwin D. Dobbs, University of Texas at Austin
James E. Boggs
Alan H. Cowley
10. New, Unsaturated Three- and Four-Membered Rings: Formal Addition of CH_2, SiH_2, GeH_2, or SnH_2 to Phoshaalkyne Triple Bonds.

Donald B. Boyd, Eli Lilly and Company
David W. Smith
James J. P. Stewart, United States Air Force Academy
Erich Wimmer, Cray Research
11. Importance of Criteria for Self-Consistent Field Convergence and Geometry Optimization in AM1, MNDO, and MINDO/3 Molecular Orbital Calculations.

William J. Welsh, University of Missouri, St. Louis
Eric Towler
Mary Dudley
12. Computational Chemistry Studies of Antifolate Drugs for Treatment of Pneumocystis Carinii Pneumonia (PCP) in AIDS Patients: Trimetrexate and Analogues.

John T. Blair, Rutgers University
Karsten Krogh-Jespersen
Ronald M. Levy
13. Solute-Solvent Interactions in Ground and Excited Electronic States.

George Chang, Columbia University
Wayne C. Guida, Ciba-Geigy
W. C. Still, Columbia University
14. Examination of Monte Carlo Approaches for Analysis of Conformational Space.

Donald Bashford, Harvard University
C. Chothia, MRC Laboratory of Molecular Biology, Cambridge
A. M. Lesk
15. The Use of Sequence Templates to Investigate the Determinants of Protein Folds.

Kyoko Watanabe, University of Pennsylvania
Michael L. Klein
16. Molecular Dynamics Study of a Sodium Octanoate Micelle in Aqueous Solution.

Robert E. Bruccoleri, Massachusetts General Hospital
Jiri Novotny
Edgar Haber
17. Prediction of Polypeptide Segments Using Conformational Search.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

Michael McKee, Auburn University
18. Ab Initio Calculations on the Boron Hydrides through B_9H_{15}.

Michelle M. Francl, Bryn Mawr College
Yuh-Min Chook
19. Cis-Trans Isomerization of Alkenyl Aluminum Complexes.

Janet Cicariello, Rutgers University
Wilma K. Olson
20. Theoretical Analysis of the Long-Range Electrostatic Potential of Supercoiled DNA.

Mark A. Murcko, Merck Sharp and Dohme, West Point
21. Using Ab Initio Calculations to Develop Molecular Mechanics Parameters for Use In Biological Simulations.

Mark Froimowitz, McLean Hospital
Ahammadunny P. A.
22. Conformational Free Energies of Cyclic Enkephalin Analogs.

Donna A. Bassolino, Rutgers University
Douglas B. Kitchen
Dorothea Kominos
Arthur Pardi
Ronald M. Levy
23. New Methods for the Refinement of Protein Structures Generated from Solution NMR Data: Application to Rabbit Neutrophil Polypeptide (NP-5).

Byungkook Lee, National Institutes of Health
24. Thermodynamics of Solvent Reorganization Upon Dissolution of Hydrocarbon Solutes in Aqueous and Hydrocarbon Solvents.

Daniel A. Kleier, Dupont
25. The Role of Electronic Structure Calculations in Optimizing the Activity of a New Class of Photosystem I Herbicides.

Peter D. J. Grootenhuis, Organon
Peter A. Kollman, University of California, San Francisco
26. Free Energy Calculations on Molecular Host-Guest Complexes.

Marcus E. Brewster, Pharmatec
James J. Kaminski, University of Florida, College of Pharmacy
Nicholas Bodor
27. Hydride Transfer Between 1-Methyl-1,4-dihydronicotinamide and the 1-Methylnicotinamide Cation, A Theoretical Study.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

T. J. O'Donnell, National Center for Supercomputing Applications
John S. Garavelli, University of Illinois at Chicago
28. A Proposal for a Standard Format for Molecular Description Files.

James J. P. Stewart, United States Air Force Academy
29. Re-Optimization of Parameters for MNDO.

John McKelvey, Eastman Kodak, Rochester
30. Quick-Pi: A Generalized Omega Method.

July 5, 1988
Tuesday Morning 9:00 a.m. - 12:05 p.m.

Norman L. Allinger, University of Georgia
Session Chairman and Discussion Leader
Molecular Mechanics.

Tommy Liljefors, University of Lund
Molecular Mechanics in Structure-Activity Studies.

Coffee break 10:05 - 10:35 a.m.

W. Clark Still, Columbia University
Modeling of Molecular Complexes.

Thomas A. Halgren, Merck Sharp and Dohme, Rahway
On the Representation of Angle Bending Potentials in Empirical Force Fields.

Tuesday Evening 7:30 p.m. - 9:20 p.m.

Yoshikazu Oka, Takeda Chemical Industries
Session Chairman and Discussion Leader
Molecular Modeling in the Chemical and Pharmaceutical Industries of Japan.

Klaus Mueller, Hoffmann-LaRoche, Basel
Combined Use of Computer Modeling and Structural Databases in Chemical Research.

Robert S. Pearlman, University of Texas, College of Pharmacy
Rapid Generation of High Quality Approximate 3D Molecular Structures.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

July 6, 1988
Wednesday Morning 9:00 a.m. - 12:05 p.m.

William L. Jorgensen, Purdue University
Session Chairman and Discussion Leader
Macromolecular Simulations.

Nobuhiro Go, Kyoto University
Simulation of Conformational Dynamics of Proteins: Harmonic and Anharmonic Aspects.

Coffee break 10:05 - 10:35 a.m.

Shoshana J. Wodak, Universite Libre de Bruxelles
Contributions from Electronic Polarizability to Electrostatic Interactions in Proteins.

Stephen H. Bryant, Brookhaven National Laboratory
Energy Functions from the Database of Known Protein Structures?

Wednesday Evening Poster Session
7:30 p.m. - 9:30 p.m.

Volker Buss, Universitat Duisburg
Peter Faupel
1. Evidence for, and Proposed Structure of, a New Folded Conformation of Methotrexate.

Keerthi Jayasuriya, Picatinny Arsenal
Sury Iyer
2. A Computational Analysis of Ortho-lithiation Reaction Mechanism.

Gerhard Barnickel, E. Merck, Darmstadt
3. Conversion Tools for Connection between Different Force-Field Programs Using CPECM.

Francesc Manaut, Institut Municipal d'Investigacio Medica, Barcelona
J. Jose
F. Sanz
4. Automatic Search of Maximum Similarity between Molecular Electrostatic Potential Distributions.

Nick C. Perry, Chemical Design Ltd., Oxford
5. A Multivariate QSAR Study on Histamine H_2 Antagonist Activity Using Structural Parameters Determined by Molecular Modelling.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

Scott G. Wierschke, Wright-Patterson Air Force Base
6. A Computational Study of the Tensile and Compressive Properties of Ordered Polymers via the Austin Model 1 (AM1) Semiempirical Molecular Orbital Method.

Jorge A. Medrano, Buenos Aires University
Roberto C. Bochicchio
Hector F. Reale
7. On the Extension of the Quantum Theory of Valence and Bonding to Periodic Systems.

Ingrid Pettersson, Royal Danish School of Pharmacy
Tommy Liljefors, University of Lund
Klaus Bogeso, Lundbeck A/S, Denmark
8. Conformational Analysis of Some D-1 Dopamine Receptor Agonists and Antagonists.

Flemming Steen Jorgensen, Royal Danish School of Pharmacy
9. Muscarinic Agonists - Towards a Common Pharmacophore Model for Enantiomers with Very Different Biological Potency.

Carol A. Venanzi, New Jersey Institute of Technology
Krishnan Namboodiri, Naval Research Laboratory
10. Structure-Function Relationships in Artificial Enzymes.

Thomas J. Venanzi, College of New Rochelle
Carol A. Venanzi, New Jersey Institute of Technology
11. Electrostatic Potential Patterns of Amiloride Analogs.

M. Katharine Holloway, Merck Sharp and Dohme, West Point
Kenneth M. Merz, University of California, San Francisco
Charles H. Reynolds, Rohm and Haas
12. A Theoretical Study of the Azophenine Potential Surface.

Sandor Vajda, Mount Sinai School of Medicine
Istvan P. Sugar
C. DeLisi
13. Combinatorial Optimization Methods for Predicting the Backbone Structure in Polypeptides.

Robin J. Breckenridge, Sandoz, Basel
Hans-Peter Weber
14. Tertiary Conformation of Marine Snail alpha-Conotoxin: Strategy for Conformational Searching Using Molecular Dynamics.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

Stephen R. Wilson, New York University
Jules W. Moskowitz
Kevin E. Schmidt
Weili Cui
15. Applications of Simulated Annealing to the Conformational Analysis of Flexible Molecules.

Renee L. DesJarlais, University of California, San Francisco
Brian Shoichet
Dale Bodian
George L. Seibel
Irwin D. Kuntz, Jr.
16. A Second Generation Computer-Assisted Inhibitor Design Method.

Martin Head-Gordon, Carnegie-Mellon University
John A. Pople
17. A New Method For Two Electron Integral Evaluation.

Kevin E. Gilbert, Indiana University, Bloomington
J. J. Gajewski
T. W. Kreek
18. Molecular Mechanics and Transition Metal Complexes.

Alan H. Katz, Wyeth-Ayerst
19. An On-Line System to Guide the Chemist in Using Computational Chemistry Software.

DeLos F. DeTar, Florida State University
20. Toward Standards for Force Field Representation.

Paul Weiner, Alliant
Roberto Gomberts
Nick Camp
21. Parallel Processing in Computational Chemistry.

Regine Snay Bohacek, Ciba-Geigy
Robert Jernigan, National Institutes of Health
22. Configurational Statistics of Methyl Vinyl Ether-Maleic Anhydride Copolymer.

Frank H. Clarke, Ciba-Geigy
23. Partition Coefficients of Ions: Determination of Distribution Profiles.

M. Rami Reddy, University of North Carolina at Chapel Hill
Max Berkowitz
24. Hydration Forces between Parallel DNA Double Helices: Computer Simulations.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

T. A. Halgren, Merck Sharp and Dohme, Rahway
B. L. Bush
25. The Use of Enzyme Site Maps in Designing Enzyme Inhibitors.

Richard D. Cramer III, Tripos Associates
David E. Patterson
Jeffrey D. Bunce
26. Comparative Molecular Field Analysis (CoMFA).

July 7, 1988
Thursday Morning 9:00 a.m. - 12:05 p.m.

Werner Braun, Eidgenossische Technische Hochschule, Zurich
Session Chairman and Discussion Leader
Distance Geometry.

Irwin D. Kuntz, Jr., University of California, San Francisco
Use of Distance Geometry for Structural Analysis.

Coffee break 10:05 - 10:35 a.m.

Jeffrey M. Blaney, Dupont
Distance Geometry Approach to Ligand-Macromolecule Docking.

J. Scott Dixon, Smith Kline and French
Ligand Design Methodology.

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

Thursday Dinner: New England Buffet

Thursday Evening 7:30 p.m. - 9:20 p.m.

Kendall N. Houk, National Science Foundation
Session Chairman and Discussion Leader
Transition Structures of Pericyclic Reactions.

Michael J. S. Dewar, University of Texas
Use of Quantum Mechanical Models for Studies of Reaction Mechanisms.

John A. Pople, Carnegie-Mellon University
General Theory of Molecular Energies.

July 8, 1988
Friday Morning 8:50 a.m. - 11:45 a.m.

Stelian Grigoras, Dow Corning
Session Chairman and Discussion Leader
Polymer Conformation in Liquid and Solid State.

Michael C. Zerner, University of Florida
Quantum Chemical Studies on the Structure and Spectroscopy of Large Transition Metal Systems.

Coffee break 9:55 - 10:15 a.m.

Joseph W. Lauher, State University of New York, Stony Brook
Molecular Modeling in Organometallic Chemistry.

Jeremy K. Burdett, University of Chicago
Theoretical Studies of Solids.

Acknowledgments
Gordon Research Conference Board of Trustees
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Quantum Chemistry Program Exchange, Indiana University
Eli Lilly and Company
University of California, San Francisco

Session Chairmen will have 15 minutes for their presentations plus 5 minutes for open discussion.
Speakers will have 35 minutes for their presentations plus 10 minutes for open discussion.

GORDON CONFERENCE ON COMPUTATIONAL CHEMISTRY

CHANGES IN THE POSTER PROGRAM

MONDAY EVENING

31. TERRY STOUCH: CRYSTAL SIMULATIONS OF LIPIDS

12. add to current poster 12: LINDA MCMILLAN and W.J. WELSH: COMPUTATIONAL CHEMISTRY STUDIES OF ANTINEOPLASTIC ANTIFOLATES

WEDNESDAY EVENING

Posters 6 and 7 on the previous schedule are cancelled.

6. LORNE REID: BUILDING BLOCKS AND PROTEIN MODELS

7. STEVE BRYANT: PACKING INTERACTIONS IN BETA ALPHA BETA PROTEINS

27. DAVID PEARLMAN: FREE ENERGY CALCULATIONS: AT WHAT COST?

28. JOHN BADGER: CRYSTALLOGRAPHIC AND COMPUTATIONAL STUDIES OF DRUG BINDING TO HUMAN RHINOVIRUS

29. JOE LAUHER: DESIGNING MOLECULAR SOLVENTS

30. AMIL ANDERSON AND JAN HERMANS: MOLECULAR DYNAMICS DERIVED FREE ENERGIES MAPS FOR HYDRATED MODEL PEPTIDES

31. GERHARD KLEBE and HANS BEAT BURGI: SYSTEMATICS IN CHEMICAL BONDING INVESTIGATED BY THE STATISTICAL EVALUATION OF STRUCTURAL DATA: BOND LENGTH VARIATION IN THE TRIGONAL BIPYRAMID

GORDON RESEARCH CONFERENCES
COMPUTATIONAL CHEMISTRY

Donald B. Boyd and Peter Kollman, Co-chairmen
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Plymouth, New Hampshire
July 4-8, 1988

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